

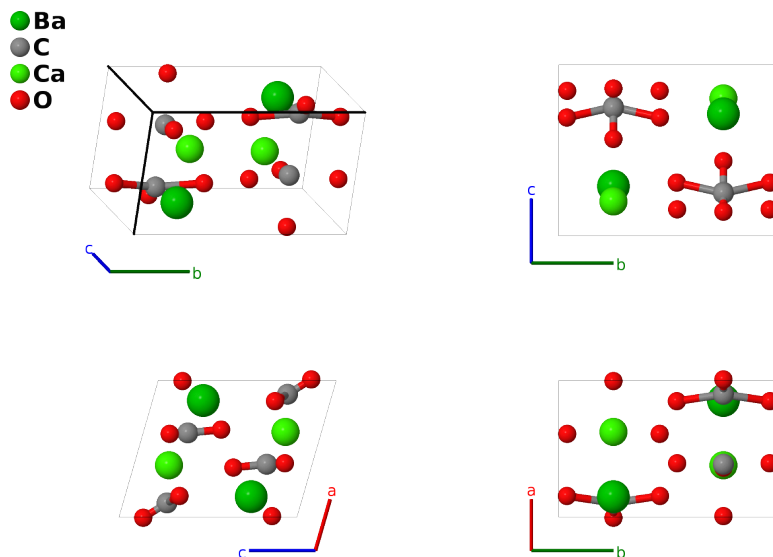
# Barytocalcite ( $\text{BaCa}(\text{CO}_3)_2$ ) Structure: AB2CD6\_mP20\_11\_e\_2e\_e\_2e2f-001

This structure originally had the label AB2CD6\_mP20\_11\_e\_2e\_e\_2e2f. Calls to that address will be redirected here.

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<https://aflow.org/p/YSME>

[https://aflow.org/p/AB2CD6\\_mP20\\_11\\_e\\_2e\\_e\\_2e2f-001](https://aflow.org/p/AB2CD6_mP20_11_e_2e_e_2e2f-001)



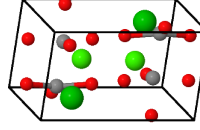
Prototype	$\text{BaC}_2\text{CaO}_6$
AFLOW prototype label	AB2CD6_mP20_11_e_2e_e_2e2f-001
Mineral name	barytocalcite
ICSD	none
Pearson symbol	mP20
Space group number	11
Space group symbol	$P2_1/m$
AFLOW prototype command	<pre>aflow --proto=AB2CD6_mP20_11_e_2e_e_2e2f-001 --params=a,b/a,c/a,beta,x1,z1,x2,z2,x3,z3,x4,z4,x5,z5,x6,z6,x7,y7,z7,x8,y8,z8</pre>

- $\text{BaCa}(\text{CO}_3)_2$  comes in a variety of crystal structures (Spahr, 2019):
  - monoclinic barytocalcite, space group  $P2_1/m$  #11 (the current structure)
  - trigonal paralstonite, space group  $P321$  #150,
  - triclinic alstonite (space group  $P1$  #1 or  $P\bar{1}$  #2) (Sartori, 1975), and
  - a new monoclinic structure, space group  $C2$  #5, synthesized by (Spahr, 2019) and lacking the centrosymmetric character of barytocalcite.

## Simple Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$

$a_3$   $a_1$   
 $a_2$



## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2e)	Ba I
$\mathbf{B}_2$	$-x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(2e)	Ba I
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2e)	C I
$\mathbf{B}_4$	$-x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(2e)	C I
$\mathbf{B}_5$	$x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2e)	C II
$\mathbf{B}_6$	$-x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(2e)	C II
$\mathbf{B}_7$	$x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2e)	Ca I
$\mathbf{B}_8$	$-x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(2e)	Ca I
$\mathbf{B}_9$	$x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(2e)	O I
$\mathbf{B}_{10}$	$-x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(2e)	O I
$\mathbf{B}_{11}$	$x_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(2e)	O II
$\mathbf{B}_{12}$	$-x_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(2e)	O II
$\mathbf{B}_{13}$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4f)	O III
$\mathbf{B}_{14}$	$-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4f)	O III
$\mathbf{B}_{15}$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4f)	O III
$\mathbf{B}_{16}$	$x_7 \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4f)	O III
$\mathbf{B}_{17}$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(4f)	O IV
$\mathbf{B}_{18}$	$-x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$	=	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(4f)	O IV
$\mathbf{B}_{19}$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	=	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(4f)	O IV
$\mathbf{B}_{20}$	$x_8 \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(4f)	O IV

## References

- [1] B. Dickens and J. S. Bowen, *The Crystal Structure of BaCa(CO<sub>3</sub>)<sub>2</sub> (barytocalcite)*, J. R. Nat. Bur. Stand. A **75**, 197–203 (1971), doi:10.6028/jres.075A.020.
- [2] F. Sartori, *New data on alstonite*, Lithos **8**, 199–207 (1975).

## Found in

- [1] D. Spahr, L. Bayarjargal, V. Vinograd, R. Luchitskaia, V. Milman, and B. Winkler, *A new  $BaCa(CO_3)_2$  polymorph*, Acta Crystallogr. Sect. B **75**, 291–300 (2019), doi:10.1107/S2052520619003238.